

Specifics of impurity effects in ferropnictide superconductors

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Effects of impurities and disorder on quasiparticle spectrum in superconducting iron pnictides are considered. Possibility for occurrence of localized energy levels due to impurities within the superconducting gap and the related modification of band structure and of superconducting order parameter are discussed. The evolution of superconducting state with impurity doping is traced.

PACS numbers: 74.70.Xa, 74.62.-c, 74.62.Dh, 74.62.En

I. INTRODUCTION

The recent discovery of superconductivity (SC) with rather high critical temperature in the family of doped ferropnictide compounds [1, 2], has motivated a great interest to these materials. Unlike the extensively studied cuprate family [3], that present insulating properties in their initial undoped state, the undoped LaOFeAs compound is a semimetal. The scanning tunnel microscopy (STM) study [4] established that this material has a layered structure, where the relevant for SC layer is FeAs with a 2D square lattice by Fe atoms and with As atoms located out of plane, above or below the centers of square cells (Fig. 1). Its electronic structure, relevant for constructing microscopic SC models, have been explored with high-resolution angle-resolved photoemission spectroscopy (ARPES) techniques [5, 6]. Their results indicate the multiple connected structure of Fermi surface, consisting of electron and hole pockets and absence of nodes in both electron and hole gaps [5], suggesting these systems to display the so-called extended *s*-wave SC order, changing its sign between electron and hole segments [10].

To study the band structure, the first principles numeric calculations are commonly used, outlining the importance of Fe atomic *d*-orbitals. The calculations show that SC in these materials is associated with Fe atoms in the layer plane, represented in Fig. 1 by their orbitals and the related hopping amplitudes. The dominance of Fe atomic 3*d* orbitals in the density of states of LaOFeAs compound near its Fermi surface was demonstrated by the local density approximation (LDA) calculations [7–12]. It was then concluded that the multi-orbital effects are important for electronic excitation spectrum in the SC state, causing formation of two gaps: by electron and hole pockets at the Fermi surface. To explain the observed SC properties, it is suggested that these materials may reveal an unconventional pairing mechanism, beyond the common electron-phonon scheme [13, 14]. In general, the total of 5 atomic orbitals for each iron in the LaOFeAs compound can be involved, however the ways

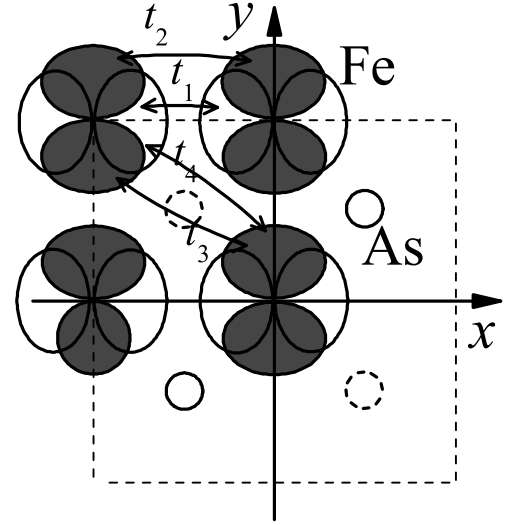


FIG. 1: Schematics of a FeAs layer in the LaOFeAs compound with d_{xz} (white) and d_{yz} (dark) Fe orbitals and the Fe-Fe hopping parameters in the minimal coupling model. Note that the hoppings between next near neighbors ($t_{3,4}$) are mediated by the As orbitals (out of Fe plane).

to reduce this basis are sought, in order to simplify analytical and computational work. Some authors [15, 16] have suggested that it is sufficient to consider only the d_{xz} and d_{yz} orbitals. Thus, building such minimal coupling model based on two orbitals, one is able to adjust the model parameters (energy hopping and chemical potential) to obtain the Fermi surface with the same topology that found in the first principles calculations of band structure.

Having established the SC state parameters, an important class of problems can be considered about the effects of disorder, in particular by impurities, on the system electronic properties, and this issue has been also studied for doped ferropnictides. Alike the situation in doped perovskite cuprates, here impurity centers can either result from the dopants, necessary to form the very superconducting state, or from foreign atoms and other

local defects in the crystalline structure. Within the minimal coupling model, an interesting possibility for localized impurity levels to appear within SC gaps in doped LaOFeAs was indicated, even for the simplest, so-called isotopic (or non-magnetic) type of impurity perturbation [17, 18]. This finding marks an essential difference from the traditional SC systems with s -wave gap on a single-connected Fermi surface, where such perturbations are known not to produce localized impurity states and thus to have no sizeable effect on SC transition temperature, accordingly to the Anderson theorem [19]. In presence of localized quasiparticle states by isolated impurity centers, the next important issue is the possibility for collective behavior of such states at high enough impurity concentrations. This possibility was studied long ago for electronic quasiparticles in doped semiconducting systems [20] and also for other types of quasiparticles in p-nonic, magnonic, excitonic, etc. spectra under impurities [21], establishing conditions for collective (including coherent) behavior of impurity excitations with striking effects in observable properties of such systems. As to the high- T_c doped cuprates, it is known that their d -wave symmetry of SC order only permits existence of impurity resonances [22, 23], not the true localization, and hinders notable collective effects on their observable properties. As to our knowledge, no consistent study on collective impurity effects is known for the doped ferropnictide systems up to the moment, and this defines the main emphasis of the present work. Namely, we shall develop an analysis of these systems, using the Green function (GF) techniques, similar to those for doped cuprate SC systems [24], the minimal coupling model by two orbitals for ferropnictide electronic structure, and the simplest isotopic type for impurity perturbation. The structure of quasiparticle spectrum near in-gap impurity levels at finite impurity concentrations, conditions for emergence of specific branches of collective excitations in this region of the spectrum, and expected observable effects of such spectrum restructuring will be discussed.

II. MODEL HAMILTONIAN AND GREEN FUNCTIONS

For the minimal coupling model of Fig. 1, the hopping Hamiltonian H_t is written in the local orbital basis as:

$$\begin{aligned}
 H_t = & - \sum_{\mathbf{n}, \sigma} [t_1 (x_{\mathbf{n}, \sigma}^\dagger x_{\mathbf{n}+\delta_x, \sigma} + y_{\mathbf{n}, \sigma}^\dagger y_{\mathbf{n}+\delta_y, \sigma} + h.c.) \\
 & + t_2 (x_{\mathbf{n}, \sigma}^\dagger x_{\mathbf{n}+\delta_y, \sigma} + y_{\mathbf{n}, \sigma}^\dagger y_{\mathbf{n}+\delta_x, \sigma} + h.c.) \\
 & + t_3 (x_{\mathbf{n}, \sigma}^\dagger x_{\mathbf{n}+\delta_x+\delta_y, \sigma} + x_{\mathbf{n}, \sigma}^\dagger x_{\mathbf{n}+\delta_x-\delta_y, \sigma} \\
 & + y_{\mathbf{n}, \sigma}^\dagger y_{\mathbf{n}+\delta_x+\delta_y, \sigma} + y_{\mathbf{n}, \sigma}^\dagger y_{\mathbf{n}+\delta_x-\delta_y, \sigma} + h.c.) \\
 & + t_4 (x_{\mathbf{n}, \sigma}^\dagger y_{\mathbf{n}+\delta_x+\delta_y, \sigma} + y_{\mathbf{n}, \sigma}^\dagger x_{\mathbf{n}+\delta_x+\delta_y, \sigma} \\
 & - x_{\mathbf{n}, \sigma}^\dagger y_{\mathbf{n}+\delta_x-\delta_y, \sigma} - y_{\mathbf{n}, \sigma}^\dagger x_{\mathbf{n}+\delta_x-\delta_y, \sigma} + h.c.)]. \quad (1)
 \end{aligned}$$

where $x_{\mathbf{n}, \sigma}$ and $y_{\mathbf{n}, \sigma}$ are the Fermi operators for d_{xz} and d_{yz} Fe orbitals with spin σ on \mathbf{n} lattice site and the

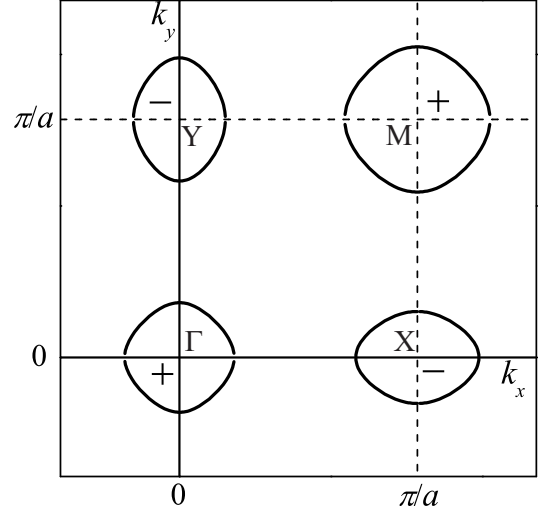


FIG. 2: Electron (-) and hole (+) segments of the Fermi surface in the normal state of model system with electronic spectrum by Eq. 5. The center of first Brillouin zone is displaced by $(\pi/2a, \pi/2a)$ to fully include all the segments around four characteristic points Γ , X , M , and Y in this zone.

vectors $\delta_{x,y}$ point to its nearest neighbors in the square lattice. Passing to the operators of orbital plane waves $x_{\mathbf{k}, \sigma} = N^{-1/2} \sum_{\mathbf{n}} e^{i\mathbf{k} \cdot \mathbf{n}} x_{\mathbf{n}, \sigma}$ (with the number N of lattice cells) and analogous $y_{\mathbf{k}, \sigma}$, and defining an "orbital" 2-spinor $\psi^\dagger(\mathbf{k}, \sigma) = (x_{\mathbf{k}, \sigma}, y_{\mathbf{k}, \sigma})$, one can expand the spinor Hamiltonian in quasimomentum:

$$H_t = \sum_{\mathbf{k}, \sigma} \psi^\dagger(\mathbf{k}, \sigma) \hat{h}_t(\mathbf{k}) \psi(\mathbf{k}, \sigma). \quad (2)$$

Here the 2×2 matrix

$$\hat{h}_t(\mathbf{k}) = \varepsilon_{+, \mathbf{k}} \hat{\sigma}_0 + \varepsilon_{-, \mathbf{k}} \hat{\sigma}_3 + \varepsilon_{xy, \mathbf{k}} \hat{\sigma}_1 \quad (3)$$

includes the Pauli matrices $\hat{\sigma}_i$ and the energy functions

$$\varepsilon_{\pm, \mathbf{k}} = \frac{\varepsilon_{x, \mathbf{k}} \pm \varepsilon_{y, \mathbf{k}}}{2},$$

with

$$\begin{aligned}
 \varepsilon_{x, \mathbf{k}} &= -2t_1 \cos k_x - 2t_2 \cos k_y - 4t_3 \cos k_x \cos k_y, \\
 \varepsilon_{y, \mathbf{k}} &= -2t_1 \cos k_y - 2t_2 \cos k_x - 4t_3 \cos k_x \cos k_y, \\
 \varepsilon_{xy, \mathbf{k}} &= -4t_4 \sin k_x \sin k_y. \quad (4)
 \end{aligned}$$

An optimum fit for the calculated band structure within the minimum coupling model is attained with the following set of hopping parameters (in $|t_1|$ units): $t_1 = -1.0$, $t_2 = 1.3$, $t_3 = t_4 = -0.85$, and with the choice of the Fermi energy (chemical potential at zero temperature) $\varepsilon_F = 1.45$ [12]. The \hat{h}_t matrix is diagonalized by the standard unitary transformation:

$$\hat{U}(\mathbf{k}) = \begin{pmatrix} \cos \theta_{\mathbf{k}}/2 & -\sin \theta_{\mathbf{k}}/2 \\ \sin \theta_{\mathbf{k}}/2 & \cos \theta_{\mathbf{k}}/2 \end{pmatrix},$$

with $\theta_{\mathbf{k}} = \arctan(\varepsilon_{xy,\mathbf{k}}/\varepsilon_{-, \mathbf{k}})$, transforming from the orbital to subband basis:

$$\hat{h}_b(\mathbf{k}) = \hat{U}^\dagger(\mathbf{k})\hat{h}_t(\mathbf{k})\hat{U}(\mathbf{k}) = \begin{pmatrix} \varepsilon_{e,\mathbf{k}} & 0 \\ 0 & \varepsilon_{h,\mathbf{k}} \end{pmatrix} \quad (5)$$

The energy eigenvalues in Eq. 4:

$$\varepsilon_{h,e}(\mathbf{k}) = \varepsilon_{+, \mathbf{k}} \pm \sqrt{\varepsilon_{xy,\mathbf{k}}^2 + \varepsilon_{-, \mathbf{k}}^2}, \quad (6)$$

correspond to the two subbands in the normal state spectrum that respectively define electron and hole pockets of the Fermi surface. There are two segments of each type, defined by the equations $\varepsilon_{e,h}(\mathbf{k}) = \mu$, as shown in Fig. 2. We note that both functions $\cos\theta_{\mathbf{k}}$ and $\sin\theta_{\mathbf{k}}$ change their sign around these segments, corresponding to their "azimuthal dependencies" around characteristic points of the Brillouin zone (Fig. 2), so that integrals of these functions with some azimuthal-independent factors over the relevant vicinity of Fermi surface practically vanish and are neglected beside such integrals of fully azimuthal-independent functions in the analysis below.

The adequate basis for constructing the SC state is generated by the operators of electron and hole subbands:

$$\begin{aligned} \alpha_{\mathbf{k},\sigma} &= x_{\mathbf{k},\sigma} \cos\theta_{\mathbf{k}}/2 - y_{\mathbf{k},\sigma} \sin\theta_{\mathbf{k}}/2, \\ \beta_{\mathbf{k},\sigma} &= y_{\mathbf{k},\sigma} \cos\theta_{\mathbf{k}}/2 + x_{\mathbf{k},\sigma} \sin\theta_{\mathbf{k}}/2, \end{aligned} \quad (7)$$

giving rise to the "multiband-Nambu" 4-spinors $\Psi_{\mathbf{k}}^\dagger = (\alpha_{\mathbf{k},\uparrow}^\dagger, \alpha_{-\mathbf{k},\downarrow}^\dagger, \beta_{\mathbf{k},\uparrow}^\dagger, \beta_{-\mathbf{k},\downarrow}^\dagger)$ and to a 4×4 extension of the Hamiltonian Eq. 2 in the form:

$$H_s = \sum_{\mathbf{k},\sigma} \Psi_{\mathbf{k}}^\dagger \hat{h}_s(\mathbf{k}) \Psi_{\mathbf{k}}, \quad (8)$$

where the 4×4 matrix

$$\hat{h}_s(\mathbf{k}) = \hat{h}_b(\mathbf{k}) \otimes \hat{\tau}_3 + \Delta_{\mathbf{k}} \hat{\sigma}_0 \otimes \hat{\tau}_1,$$

includes the Pauli matrices $\hat{\tau}_i$ acting on the Nambu (particle-antiparticle) indices in Ψ -spinors and $\hat{h}_b(\mathbf{k})$ is defined by Eq. 5. The simplified form for the extended s -wave SC order is realized with the definition of the gap function by constant values, $\Delta_{\mathbf{k}} = \Delta$ on the electron segments and $\Delta_{\mathbf{k}} = -\Delta$ on the hole segments.

The electronic dynamics of this system is determined by the (Fourier transformed) GF 4×4 matrices [21, 24, 25]:

$$\hat{G}_{\mathbf{k},\mathbf{k}'} = \langle \langle \Psi_{\mathbf{k}} | \Psi_{\mathbf{k}'}^\dagger \rangle \rangle = i \int_{-\infty}^0 dt e^{i\varepsilon t/\hbar} \langle \{ \Psi_{\mathbf{k}}(t), \Psi_{\mathbf{k}'}^\dagger(0) \} \rangle, \quad (9)$$

whose energy argument ε is understood as $\varepsilon - i0$ and $\langle \{ A(t), B(0) \} \rangle$ is the quantum statistical average with Hamiltonian H of the anticommutator of Heisenberg operators. From the equation of motion:

$$\varepsilon \hat{G}_{\mathbf{k},\mathbf{k}'} = \hbar \delta_{\mathbf{k},\mathbf{k}'} \hat{\sigma}_0 \otimes \tau_0 + \langle \langle [\Psi_{\mathbf{k}}, H] | \Psi_{\mathbf{k}'}^\dagger \rangle \rangle, \quad (10)$$

the explicit GF for the unperturbed SC system with the Hamiltonian H_s , Eq. 7, is diagonal in quasimomentum, $\hat{G}_{\mathbf{k},\mathbf{k}'} = \delta_{\mathbf{k},\mathbf{k}'} \hat{G}_{\mathbf{k}}^0$ and

$$\begin{aligned} \hat{G}_{\mathbf{k}}^0 &= \frac{\varepsilon \hat{\tau}_0 + \varepsilon_e(\mathbf{k}) \hat{\tau}_3 + \Delta \hat{\tau}_1}{2D_{e,\mathbf{k}}} \otimes \hat{\sigma}_+ \\ &+ \frac{\varepsilon \hat{\tau}_0 + \varepsilon_h(\mathbf{k}) \hat{\tau}_3 - \Delta \hat{\tau}_1}{2D_{h,\mathbf{k}}} \otimes \hat{\sigma}_-, \end{aligned} \quad (11)$$

where $\hat{\sigma}_\pm = (\hat{\sigma}_0 \pm \hat{\sigma}_3)/2$ and the secular denominators $D_{i,\mathbf{k}} = \varepsilon^2 - \varepsilon_i^2(\mathbf{k}) - \Delta^2$ for $i = e, h$. In what follows, we use the energy reference to the Fermi level ε_F and approximate the segments of Fermi surface by some circles of radius k_i around the characteristic points \mathbf{K}_i in the Brillouin zone, so that the dispersion laws $\varepsilon_j(\mathbf{k}) = \varepsilon_F + \xi_{j,\mathbf{k}}$ permit to linearize the quasiparticle dispersion close to the Fermi level as $\xi_{j,\mathbf{k}} \approx \hbar v_j (|\mathbf{k} - \mathbf{K}_j| - k_j)$. Generally, the Fermi wavenumbers k_j and related Fermi velocities v_j for $j = e$ and h can somewhat differ at a given choice of hopping parameters and chemical potential, but, for simplicity, we shall neglect this difference and consider their single values $k_j = k_F$ and $v_j = v_F$.

III. IMPURITY PERTURBATION AND SELF-ENERGY

We pass to the impurity problem where the above Hamiltonian is added by the perturbation terms due to non-magnetic impurities [17] on random sites \mathbf{p} in Fe square lattice with an on-site energy shift V :

$$H_{imp} = V \sum_{\mathbf{p},\sigma} (x_{\mathbf{p},\sigma}^\dagger x_{\mathbf{p},\sigma} + y_{\mathbf{p},\sigma}^\dagger y_{\mathbf{p},\sigma}). \quad (12)$$

Without loss of generality, the parameter V can be taken positive, and for GF calculations, this perturbation is suitably expressed in the multiband-Nambu basis:

$$H_{imp} = \frac{1}{N} \sum_{\mathbf{p},\mathbf{k},\mathbf{k}'} e^{i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{p}} \Psi_{\mathbf{k}}^\dagger \hat{V}_{\mathbf{k},\mathbf{k}'} \Psi_{\mathbf{k}'}. \quad (13)$$

through the 4×4 scattering matrix $\hat{V}_{\mathbf{k},\mathbf{k}'} = V \hat{U}_{\mathbf{k}}^\dagger \hat{U}_{\mathbf{k}'} \otimes \tau_3$. Within the approach of Refs. [21, 24], the solution for Eq. 9 with the perturbed Hamiltonian $H_s + H_i$ can be obtained in different forms, suitable for different types of states, band-like (extended) or localized. All these forms result from the basic equation of motion:

$$\hat{G}_{\mathbf{k},\mathbf{k}'} = \delta_{\mathbf{k},\mathbf{k}'} \hat{G}_{\mathbf{k}}^0 + \frac{1}{N} \sum_{\mathbf{p},\mathbf{k}''} e^{i(\mathbf{k}'' - \mathbf{k}) \cdot \mathbf{p}} \hat{G}_{\mathbf{k}}^0 \hat{V}_{\mathbf{k},\mathbf{k}''} \hat{G}_{\mathbf{k}'',\mathbf{k}'}, \quad (14)$$

by specific routines of iterating this equation for the "scattered" GF's $\hat{G}_{\mathbf{k}'',\mathbf{k}'}$.

Thus, the algorithm, where the next iteration step *never* applies to the scattered GF's already present after previous steps, e.g. that with $\mathbf{k}'' = \mathbf{k}$ in Eq. 14,

leads to the so-called fully renormalized form, suitable for band-like states:

$$\hat{G}_{\mathbf{k}} = \left[\left(\hat{G}_{\mathbf{k}}^0 \right)^{-1} - \hat{\Sigma}_{\mathbf{k}} \right]^{-1}, \quad (15)$$

where the self-energy matrix $\hat{\Sigma}_{\mathbf{k}}$ is expressed by the related group expansion (GE):

$$\hat{\Sigma}_{\mathbf{k}} = c\hat{T}_{\mathbf{k}} \left(1 + c\hat{B}_{\mathbf{k}} + \dots \right). \quad (16)$$

Here $c = \sum_{\mathbf{p}} N^{-1}$ is the impurity concentration (per Fe site) and the T-matrix results from all the multiple scatterings by a single impurity:

$$\begin{aligned} \hat{T}_{\mathbf{k}} = & \hat{V}_{\mathbf{k},\mathbf{k}} + \frac{1}{N} \sum_{\mathbf{k}' \neq \mathbf{k}} \hat{V}_{\mathbf{k},\mathbf{k}'} \hat{G}_{\mathbf{k}'}^0 \hat{V}_{\mathbf{k}',\mathbf{k}} \\ & + \frac{1}{N^2} \sum_{\mathbf{k}' \neq \mathbf{k}, \mathbf{k}'' \neq \mathbf{k}, \mathbf{k}'} \hat{V}_{\mathbf{k},\mathbf{k}'} \hat{G}_{\mathbf{k}'}^0 \hat{V}_{\mathbf{k}',\mathbf{k}''} \hat{G}_{\mathbf{k}''}^0 \hat{V}_{\mathbf{k}'',\mathbf{k}} + \dots \end{aligned} \quad (17)$$

The next term to the unity in the brackets in Eq. 14:

$$\hat{B}_{\mathbf{k}} = \sum_{\mathbf{n}} \left(\hat{A}_{\mathbf{n}} e^{-i\mathbf{k} \cdot \mathbf{n}} + \hat{A}_{\mathbf{n}} \hat{A}_{-\mathbf{n}} \right) \left(1 - \hat{A}_{\mathbf{n}} \hat{A}_{-\mathbf{n}} \right)^{-1}, \quad (18)$$

describes the effects of indirect interactions in pairs of impurities, separated by vector \mathbf{n} , in terms of interaction matrices $\hat{A}_{\mathbf{n}} = \hat{T}_{\mathbf{k}} \sum_{\mathbf{k}' \neq \mathbf{k}} e^{i\mathbf{k}' \cdot \mathbf{n}} \hat{G}_{\mathbf{k}'}^0$. Besides this restriction on summation, multiple sums in the products like $\hat{A}_{\mathbf{n}} \hat{A}_{-\mathbf{n}}$ never contain coincident quasimomenta. Eq. 18 presents the first non-trivial GE term and the rest of its terms omitted in Eq. 14 correspond to the contributions from groups of three and more impurities [21].

An alternative iteration routine for Eq. 13 applies it to *all* the scattered GF's, this results in the so-called non-renormalized form, suitable for localized states:

$$\hat{G}_{\mathbf{k}} = \hat{G}_{\mathbf{k}}^0 + \hat{G}_{\mathbf{k}}^0 \hat{\Sigma}_{\mathbf{k}}^0 \hat{G}_{\mathbf{k}}^0. \quad (19)$$

Here the non-renormalized self-energy GE: $\hat{\Sigma}_{\mathbf{k}}^0 = c\hat{T} \left(1 + c\hat{B}_{\mathbf{k}}^0 + \dots \right)$, differs from the above renormalized one by absence of restrictions in quasimomentum sums for interaction matrices $\hat{A}_{\mathbf{n}}^0 = \hat{T}_{\mathbf{k}} \sum_{\mathbf{k}'} e^{i\mathbf{k}' \cdot \mathbf{n}} \hat{G}_{\mathbf{k}'}^0$ and their products.

At the first step, we shall restrict GE to the common T-matrix level, providing the conditions for localized quasiparticle states with in-gap energy levels to appear at single impurities [16], and will study certain (narrow) energy bands of specific collective states that can be formed near these levels at finite impurity concentrations. At the next step, the criteria for such collective states to really exist in the disordered SC system will follow from the analysis of non-trivial GE terms. We notice that presence of renormalized GF's $\hat{G}_{\mathbf{k}'}$ in the above interaction matrices is just necessary for adequate treatment of interaction effects over the in-gap bands.

IV. T-MATRIX AND QUASIPARTICLE STATES

The T-matrix, Eq. 16, is readily simplified taking into account that $\hat{V}_{\mathbf{k},\mathbf{k}} = V\hat{\sigma}_0 \otimes \hat{\tau}_3$ and introducing the integrated Green function matrix:

$$\hat{G}_0 = \frac{1}{N} \sum_{\mathbf{k}} \hat{U}_{\mathbf{k}} \hat{G}_{\mathbf{k}}^0 U_{\mathbf{k}}^\dagger = \varepsilon [g_e(\varepsilon)\hat{\sigma}_+ + g_h(\varepsilon)\hat{\sigma}_-] \otimes \hat{\tau}_0.$$

This diagonal form follows directly from the aforementioned cancellation of the integrals with $\cos \theta_{\mathbf{k}}$ and $\sin \theta_{\mathbf{k}}$ that appear in all the matrix elements of $\hat{U}_{\mathbf{k}} \hat{G}_{\mathbf{k}}^0 U_{\mathbf{k}}^\dagger$ except those proportional to $\varepsilon \hat{\sigma}_{\pm} \otimes \hat{\tau}_0$. Respectively, the functions $g_j(\varepsilon) = N^{-1} \sum_{\mathbf{k}} D_{j,\mathbf{k}}^{-1}$ for $j = e, h$ are approximated near the Fermi level, $|\varepsilon - \varepsilon_F| \lesssim \Delta$, as:

$$g_j(\varepsilon) \approx -\frac{\pi \rho_j}{\sqrt{\Delta^2 - \varepsilon^2}}. \quad (20)$$

Here $\rho_j = m_j a^2 / (2\pi \hbar^2)$ are the Fermi densities of states for respective subbands (in parabolic approximation for their dispersion laws), and by the assumed identity of all the segments of Fermi surface they can be also considered identical $\rho_j = \rho_F$. Omitted terms in Eq. 16 are of higher orders in the small parameter $|\varepsilon|/\varepsilon_F \ll 1$.

Then the momentum independent T-matrix is explicitly written as

$$\hat{T} = \gamma^2 \frac{\varepsilon - \varepsilon_0 \hat{\tau}_3}{\varepsilon^2 - \varepsilon_0^2}, \quad (21)$$

where $\varepsilon_0 = \Delta / \sqrt{1 + v^2}$ defines the in-gap impurity level [16] through the dimensionless impurity perturbation parameter $v = \pi \rho_F V$, and $\gamma^2 = v^2 V \varepsilon_0^2 / \Delta$ is the effective constant of coupling between localized and band quasiparticles.

At finite c , using this T-matrix in Eq. 14, we obtain, from the condition $\det \hat{G}_{\mathbf{k}}^{-1} = 0$ [25], the formal dispersion equation expressed through dispersion of normal quasiparticles $\xi_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \varepsilon_F$ (but in neglect of the energy level width due to the effects of indirect interaction between impurities by higher GE terms):

$$D_{\mathbf{k}}(\varepsilon) = \varepsilon^2 - \xi_{\mathbf{k}}^2 - \Delta^2 - \frac{2c\gamma^2 (\varepsilon^2 - \varepsilon_0 \xi_{\mathbf{k}})}{\varepsilon^2 - \varepsilon_0^2} = 0. \quad (22)$$

Its solutions shown in Fig. 3 in function of the quasimomentum argument $\xi = \xi_{\mathbf{k}}$ display a peculiar multiband structure. First of all, it includes four modified bands $\pm \varepsilon_b(\pm \xi)$, slightly shifted with respect to the unperturbed SC quasiparticle bands $\pm \sqrt{\Delta^2 + \xi^2}$, accordingly to the basic function:

$$\varepsilon_b(\xi) \approx \sqrt{\Delta^2 + \xi^2} + c\gamma^2 \frac{\Delta^2 + \xi^2 - \varepsilon_0 \xi}{\sqrt{\Delta^2 + \xi^2} (\xi^2 + \xi_0^2)}, \quad (23)$$

with $\xi_0^2 = \Delta^2 - \varepsilon_0^2$. It should be noted that these subbands for opposite signs of their argument ξ in fact refer to excitations around different segments (by electron and

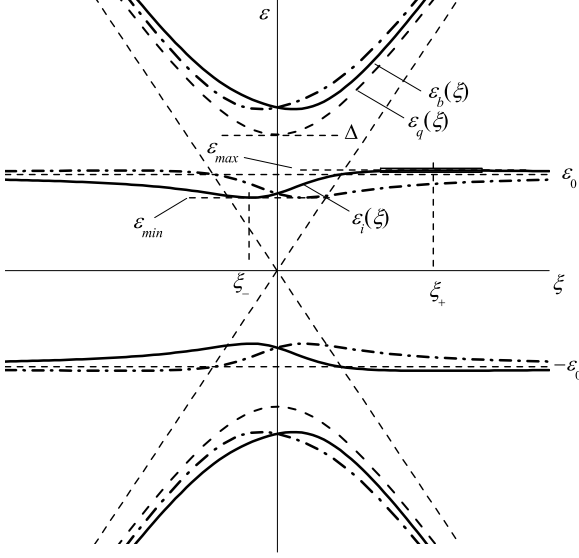


FIG. 3: Dispersion laws for band-like quasiparticles in the T-matrix approximation, neglecting their finite lifetime, at a specific choice of impurity parameters $v = 1$, $c = 0.1\Delta^2/\gamma^2$. Solid lines are for the bands near electron-like segments of Fermi surface and dash-dotted lines for those near hole-like segments. The non-perturbed SC quasiparticle bands and single-impurity localized levels are shown with dashed lines. The narrow rectangle around the top of ε_i -band delimits the region in Fig. 5.

holes) of the Fermi surface, but for clarity presented in Fig. 3 in the same ξ -reference. Besides these ε_b bands, there appear also four (narrow) in-gap bands $\pm\varepsilon_i(\pm\xi)$, generated close to $\pm\varepsilon_0$ by finite concentration of impurities, accordingly to:

$$\varepsilon_i(\xi) \approx \varepsilon_0 + c\gamma^2 \frac{\xi - \varepsilon_0}{\xi^2 + \varepsilon_0^2}, \quad (24)$$

As follows from Eq. 21, the $\varepsilon_j(\xi)$ band is located between its extrema $\varepsilon_{max} = \varepsilon_0 + c\gamma^2\varepsilon_0/(\Delta + \varepsilon_0)$ at $\xi_+ = \varepsilon_0 + \Delta$ and $\varepsilon_{min} = \varepsilon_0 - c\gamma^2\varepsilon_0/(\Delta - \varepsilon_0)$ at $-\xi_- = \varepsilon_0 - \Delta$. The energy and momentum shifts of the extremal points by Eqs. 20, 21, and Fig. 3 are specific for the impurity effect on the multiband initial spectrum and they contrast with a simpler situation for an impurity level near the edge of a single quasiparticle band [21].

All these spectrum bands would contribute to the overall density of states (DOS) by related quasiparticles: $\rho(\varepsilon) = (4\pi N)^{-1} \text{Im Tr} \sum_{\mathbf{k}} \hat{G}_{\mathbf{k}}$. The more common contributions here come from the ε_b bands and they can be expressed through the Bardeen-Cooper-Schrieffer (BCS) DOS in pure crystal [26]: $\rho_{\text{BCS}}(\varepsilon, \Delta) = \rho_F \varepsilon / \sqrt{\varepsilon^2 - \Delta^2}$,

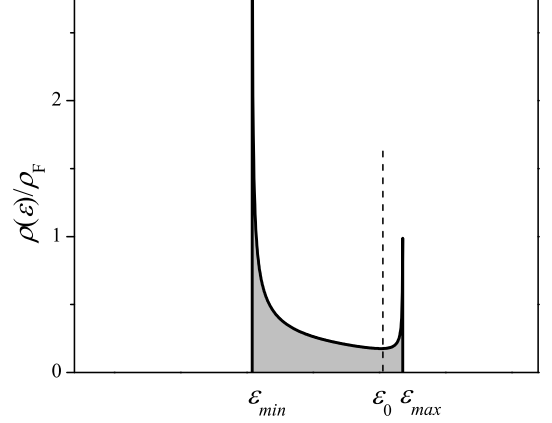


FIG. 4: Density of states in the narrow in-gap band near the impurity level ε_0 (dashed line) for the case by Fig. 3.

as follows:

$$\rho_b(\varepsilon) \approx \left(1 - \frac{c\gamma^2}{\varepsilon^2 - \varepsilon_0^2}\right) \rho_{\text{BCS}}(\varepsilon, \Delta_c), \quad (25)$$

at $\varepsilon^2 \geq \Delta_c^2 = \Delta^2 + 2c\gamma^2\varepsilon_0^2/(\Delta^2 - \varepsilon_0^2)$. The first factor in the l.h.s. of Eq. 25 describes a certain reduction of the BCS DOS, especially when the energy argument is close to the gap limits, and the shift of its gap argument is due to the quantum-mechanical repulsion between the band and impurity levels.

More peculiar is the contribution to DOS from the ε_i bands, written as:

$$\rho_i(\varepsilon) \approx \frac{\rho_F}{v} \frac{\varepsilon^2 - \varepsilon_0^2 - c\gamma^2}{\sqrt{(\varepsilon_{max}^2 - \varepsilon^2)(\varepsilon^2 - \varepsilon_{min}^2)}}, \quad (26)$$

at $\varepsilon_{min}^2 \leq \varepsilon^2 \leq \varepsilon_{max}^2$, and presented in Fig. 4.

Both the effects of ε_b band shifts and of ε_i band formation can have important repercussions in the physical behavior of the disordered SC system and they will be considered below. But before this, we need to analyze the criteria for the considered quasiparticles to really exist, especially in closeness to the limits of corresponding bands.

V. GROUP EXPANSION AND COHERENCE CRITERIA

Let us now study the crossover from band to localized states near the limits of ε_i bands, say for definiteness, its upper limit ε_{max} . Supposing the actual energy $\varepsilon < \varepsilon_{max}$ to be within the range of band states, we use the fully renormalized self-energy matrix, Eq. 16, up to the GE pair term, $c^2 \hat{T} \hat{B}_{\mathbf{k}}$, that will add a certain finite imaginary part $\Gamma_i(\xi)$ to the dispersion law $\varepsilon = \varepsilon_i(\xi)$, Eq. 23. Then

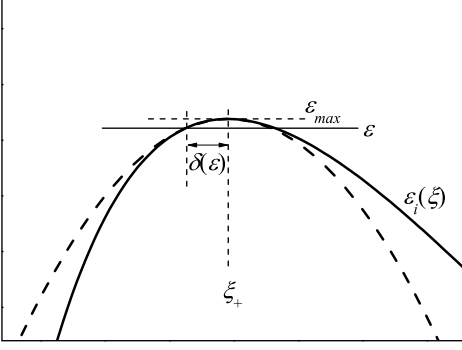


FIG. 5: Parabolic approximation (dashed line) for the dispersion law near the top of impurity band (solid line).

the known Ioffe-Regel-Mott criterion [27, 28] for the state at this energy to be really band-like (also called extended) is written as:

$$\varepsilon_{max} - \varepsilon \gg \Gamma_i(\varepsilon). \quad (27)$$

To simplify calculation of the scalar function $\Gamma_i(\varepsilon)$, we fix the energy argument in the numerators of T-matrix and interaction matrices at $\varepsilon = \varepsilon_0$, obtaining their forms:

$$\hat{T}(\varepsilon) \approx \frac{\gamma^2 \varepsilon_0}{\varepsilon^2 - \varepsilon_0^2} \hat{m}_+, \quad \hat{A}_{\mathbf{n}}(\varepsilon) \approx \hat{T}(\varepsilon) \frac{\varepsilon_0}{N} \sum_{\mathbf{k}} \frac{e^{i\mathbf{k} \cdot \mathbf{n}}}{D_{\mathbf{k}}(\varepsilon)}, \quad (28)$$

both proportional to the matrix $\hat{m}_+ = \hat{\sigma}_0 \otimes (\hat{\tau}_0 + \hat{\tau}_3)$ with important multiplicative property: $\hat{m}_+^2 = 2\hat{m}_+$. The \mathbf{k} -summation (integration) in Eq. 28 is suitable done in polar coordinates over the circular segments of Fermi surface. Here the azimuthal integration only refers to the phase of numerator, resulting in a zeroth order Bessel function: $\int_0^{2\pi} e^{ix \cos \theta} d\theta = 2\pi J_0(x)$. Since $x = n(k_F + \xi/\hbar v_F)$ is typically big, $x \gg 1$, the asymptotical formula applies: $J_0(x) \approx \sqrt{2/(\pi x)} \cos(x - \pi/4)$. Then, for radial integration in ξ around the extremum point ξ_+ , it is convenient to decompose this function in the fast and slow oscillating factors: $J_0(x) \approx \sqrt{2/(\pi k_+ n)} \cos(k_+ n - \pi/4) \cos[(\xi - \xi_+)n/\hbar v_F]$ with the fast wavenumber $k_+ = k_F + \xi_+/\hbar v_F \approx k_F$, and to write the denominator in the parabolic approximation: $D_{\xi}(\varepsilon) \approx (\xi - \xi_+)^2 - \delta^2(\varepsilon)$, with $\delta^2(\varepsilon) = 4\Delta(\Delta + \varepsilon_0)^2(\varepsilon_{max} - \varepsilon)/(2c\gamma^2)$ (see Fig. 5). Thus, the interaction matrix $\hat{A}_{\mathbf{n}}(\varepsilon) = A_n(\varepsilon)\hat{m}_+$ only depends on the distance n between impurities, and, for ε close to ε_{max} , this dependence can be expressed as:

$$A_r(\varepsilon) \approx \sqrt{\frac{r_{\varepsilon}}{r}} \sin k_{\varepsilon} r \cos k_F r, \quad (29)$$

where the length scales both for the monotonous decay:

$$r_{\varepsilon} = \frac{2\pi}{k_F} \left[\frac{\varepsilon_0 \rho_F (\Delta + \varepsilon_0)}{c\delta(\varepsilon)} \right]^2,$$

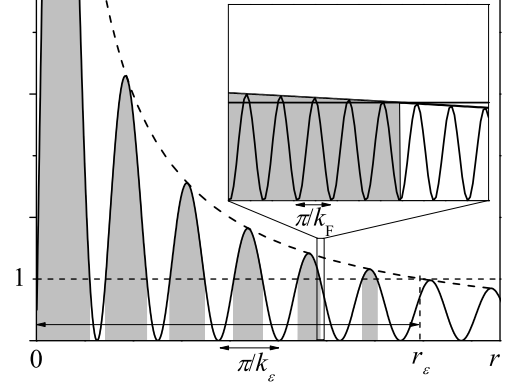


FIG. 6: Interaction function $A_r^2(\varepsilon)$ by Eq. 30 at the choice of parameters $\varepsilon_{max} - \varepsilon = 0.1$ and $\Delta/\varepsilon_F = 5 \cdot 10^{-2}$ displays slow sine oscillations (solid line) and the monotonous envelope function (dashed line). The shadowed intervals are those contributing to $\text{Im } B$, accordingly to the condition $(r_{\varepsilon}/r) \sin^2 k_{\varepsilon} r > 1$. Inset: the expansion of the rectangle in the main panel shows also fast oscillations by the cosine.

and for the sine factor: $k_{\varepsilon}^{-1} = \hbar v_F / \delta(\varepsilon)$, are much longer than k_F^{-1} for the fast cosine. The latter fast oscillation is specific for the interactions mediated by Fermi quasiparticles (like the known RKKY mechanism), unlike the monotonous or slowly oscillating interactions between impurities in semiconductors or in bosonic systems [21]. Now the calculation of $\Gamma_i(\varepsilon) = c^2 T(\varepsilon) \text{Im } B(\varepsilon)$ mainly concerns the dominant scalar part of the GE pair term:

$$B(\varepsilon) \approx \frac{2\pi}{a^2} \int_a^{r_{\varepsilon}} \frac{r dr}{1 - 4A_r^2(\varepsilon)} \quad (30)$$

(since the \mathbf{k} -dependent term in Eq. 18 turns to be negligible beside this).

The upper integration limit in Eq. 31 corresponds to the condition that its integrand only has poles for $r < r_{\varepsilon}$. In conformity with the slow and fast modes in the function, Eq. 30, the integration is naturally divided in two stages. At the first stage, integration over each m th period of fast cosine, around $r_m = 2\pi m/k_F$, is done setting constant the slow factors, $r \approx r_m$ and $\sin k_{\varepsilon} r \approx \sin k_{\varepsilon} r_m$, and using the explicit formula:

$$\text{Im} \int_{-\pi}^{\pi} \frac{dx}{1 - 4A^2 \cos^2 x} = \text{Im} \frac{\pi}{\sqrt{1 - A^2}}. \quad (31)$$

At the second stage, the summation of these results in m is approximated by the integration in the slow variable:

$$\begin{aligned} & \frac{\pi}{k_F} \text{Im} \sum_m \frac{r_m^{3/2}}{\sqrt{r_m - r_{\varepsilon} \sin^2 k_{\varepsilon} r_m}} \\ & \approx \text{Im} \int_a^{r_{\varepsilon}} \frac{r^{3/2} dr}{\sqrt{r - r_{\varepsilon} \sin^2 k_{\varepsilon} r}}. \end{aligned} \quad (32)$$

The numerical calculation of the latter integral results in:

$$\text{Im}B = \frac{r_\varepsilon^2}{a^2} f(k_\varepsilon r_\varepsilon), \quad (33)$$

where the function $f(z)$ is zero for $z < z_0 \approx 1.3585$, and monotonously grows for $z > z_0$, rapidly approaching the asymptotic constant value: $f_{as} \approx 1.1478$, for $z \gg z_0$. Then the Ioffe-Regel-Mott criterion, Eq. 27, at ε so close to ε_{max} that $k_\varepsilon r_\varepsilon \gg z_0$, is expressed as:

$$\varepsilon_{max} - \varepsilon \gg \frac{c^2 \gamma^2}{\varepsilon_{max} - \varepsilon_0} \frac{r_\varepsilon^2}{a^2}, \quad (34)$$

and this would result in a (concentration independent) estimate for the range of extended states within the impurity band:

$$\varepsilon_{max} - \varepsilon \gg \Gamma_0 = \frac{(v\varepsilon_0)^{3/2}}{ak_F} \sqrt{\frac{2\pi\rho_F}{1+v^2}}, \quad (35)$$

and its comparison with the full extension of this band, $\varepsilon_{max} - \varepsilon_{min} = c\gamma^2(1+v^2)/(v^2\Delta)$, would suggest possibility for such extended states to really exist if the impurity concentration surpass the characteristic (small) value:

$$c \gg c_0 = \frac{(\pi\rho_F\varepsilon_0)^{3/2}}{ak_F} \sqrt{\frac{2v}{1+v^2}}. \quad (36)$$

For typical values of $\rho_F^{-1} \sim 2$ eV, $ak_F \sim 1$, and $\Delta \sim 10$ meV in LaOFeAs system [5, 8, 29], and supposing a plausible impurity perturbation $v \sim 1$, we estimate $c_0 \approx 8 \cdot 10^{-4}$, manifesting important impurity effects already at their very low content.

However, the r. h. s. of Eq. 34 vanishes at $k_\varepsilon r_\varepsilon < z_0$, which occurs beyond the vicinity of the band top:

$$\varepsilon_{max} - \varepsilon > \Gamma_0 \left(\frac{c_0}{c}\right)^3. \quad (37)$$

Under the condition of Eq. 36, this vicinity is yet more narrow than Γ_0 by Eq. 35, defining the true, even wider, range of extended states.

Otherwise, for $c \ll c_0$, the impurity band does not exist, then we analyze the energy range near the impurity level with the non-renormalized GE and write the approximate criterion for its convergence as $c|B^0| \ll 1$. This calculation is done in a similar way as before but replacing the interaction function, Eq. 29, by its non-renormalized version:

$$A_r^0(\varepsilon) \approx \sqrt{R_\varepsilon/r} e^{-r/r_0} \cos k_F r, \quad (38)$$

with $k_F R_\varepsilon = 2\pi(\varepsilon_0/|\varepsilon - \varepsilon_0|)^2$ and $k_F r_0 = 2\varepsilon_F/\xi_0$. Then the above GE convergence criterion is assured beyond the following vicinity of impurity level:

$$|\varepsilon - \varepsilon_0| \gg \Gamma_c = \Gamma_0 \exp\left(-c_0^{4/3}/c\right), \quad (39)$$

defining the range of its broadening due to inter-impurity interactions. The DOS function for localized states can

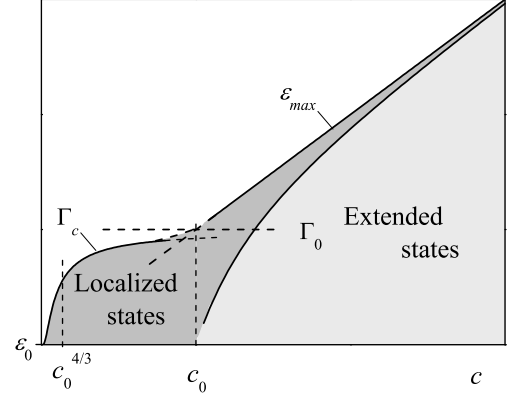


FIG. 7: Structure of the energy spectrum near the impurity level in function of impurity concentration.

be only estimated by the order of magnitude within this range, but outside is given by:

$$\begin{aligned} \rho_{loc}(\varepsilon) &\approx \frac{c^2}{c_0^{4/3} |\varepsilon - \varepsilon_0|}, \quad \text{for } \Gamma_c \ll |\varepsilon - \varepsilon_0| \ll \Gamma_0, \\ \rho_{loc}(\varepsilon) &\approx \frac{c^2 \varepsilon_0^4}{|\varepsilon - \varepsilon_0|^5}, \quad \text{for } \Gamma_0 \ll |\varepsilon - \varepsilon_0|. \end{aligned} \quad (40)$$

Notably, the total number of states near the impurity level is $\int \rho_{loc}(\varepsilon) d\varepsilon \sim c$, alike that of extended states in the impurity band by Eq. 26. The summary of evolution of this area of quasiparticle spectrum in function of impurity concentration is shown in Fig. 7.

VI. IMPURITY EFFECTS ON SC CHARACTERISTICS

The above results on the quasiparticle spectrum in the disordered SC system can be immediately used for calculation of impurity effects on its observable characteristics.

Thus the fundamental SC order parameter Δ is estimated from the modified gap equation:

$$\lambda^{-1} = \int_0^{\varepsilon_D} \rho(\varepsilon) d\varepsilon, \quad (41)$$

where $\lambda = \rho_F V_{SC}$ is the (small) dimensionless SC pairing constant and the Debye energy ε_D restricts the energy range of its action. In absence of impurities, $c = 0$, using the BCS DOS in this equation leads straightforwardly to the known result for its non-perturbed value Δ_0 : $\lambda^{-1} = \text{arcsinh}(\varepsilon_D/\Delta_0)$ and thus to $\Delta_0 \approx \varepsilon_D e^{-1/\lambda}$.

For finite c , the total DOS is combined from the contributions by the shifted main band, ρ_b , Eq. 25, and by the impurity band (or level) ρ_i (or ρ_{loc}), Eqs. 26 (or 40). The latter contribution is $\sim c$, accordingly to the previous discussion, defining a small correction beside $\lambda^{-1} \gg 1$. But

a much stronger c -dependent correction comes from the modified main band:

$$\int_{\Delta_c}^{\varepsilon_D} \rho_b(\varepsilon) d\varepsilon \approx \operatorname{arcsinh} \frac{\varepsilon_D}{\Delta_c} - c\gamma^2 \int_{\Delta_c}^{\varepsilon_D} \frac{d\varepsilon}{(\varepsilon - \varepsilon_0)^2 \sqrt{\Delta_c^2 - \varepsilon^2}}.$$

For $\varepsilon_D \gg \Delta_c$, the last integral is well approximated by:

$$c\gamma^2 \int_{\Delta_c}^{\infty} \frac{d\varepsilon}{(\varepsilon - \varepsilon_0)^2 \sqrt{\Delta_c^2 - \varepsilon^2}} = \frac{c\gamma^2}{\Delta_c^2} F\left(\frac{\Delta_c}{\varepsilon_0}\right),$$

with the function

$$F(z) = z \frac{\sqrt{z^2 - 1} + z \arccos(-1/z)}{(z^2 - 1)^{3/2}}.$$

Though this F diverges at $z \rightarrow 1$, but actually its argument

$$\Delta_c/\varepsilon_0 = \sqrt{1 + v^2} (1 + c/c_1) \quad \text{with} \quad c_1 = \pi \rho_F \Delta/v,$$

is always above unity. Neglecting the small ρ_i contribution in Eq. 41 and taking account of the BCS relation $\lambda^{-1} = \operatorname{arcsinh}(\varepsilon_D/\Delta_0)$, we express the gap equation as:

$$\operatorname{arcsinh} \frac{\Delta_c - \Delta_0}{\Delta_0} \approx \frac{cv^2}{c_1(1 + v^2)} F(\Delta_c/\varepsilon_0). \quad (42)$$

Its approximate solution for $c \ll c_1$, together with the relation: $\Delta_c/\Delta = 1 + c/[c_1(1 + v^2)]$, lead to the desired expression for the perturbed SC order parameter Δ :

$$\frac{\Delta}{\Delta_0} \approx 1 - \frac{c}{c_1} \frac{1 + v^2 F[\sqrt{1 + v^2}(1 + c/c_1)]}{1 + v^2}, \quad (43)$$

that rapidly decays with impurity concentration and would vanish at

$$c = c_1 \frac{1 + v^2}{1 + v^2 F[\sqrt{1 + v^2}(1 + c/c_1)]}.$$

The latter equality defines in fact a certain equation for c and its solution, e.g., for the above choice of $v = 1$, is $c \approx 0.5c_1 \approx 6 \cdot 10^{-3}$. However, such concentrations would already correspond to the impurity band as wide as the gap itself; this goes beyond the validity of the above derivation and needs a special treatment (to be done elsewhere).

To study another important dependence, that of the SC transition temperature T_c on concentration c , one has, strictly speaking, to extend the above GF techniques for finite temperatures, but a very simple estimate can be done, supposing that the BCS relation $\Delta/T_c \approx 1.76$ still holds in the presence of impurities. Then the r.h.s. of Eq. 43 would also describe the decay of T_c/T_{c0} .

It is of interest to compare the present results with the known Abrikosov-Gor'kov solution for BCS SC with paramagnetic impurities in the Born approximation [30,

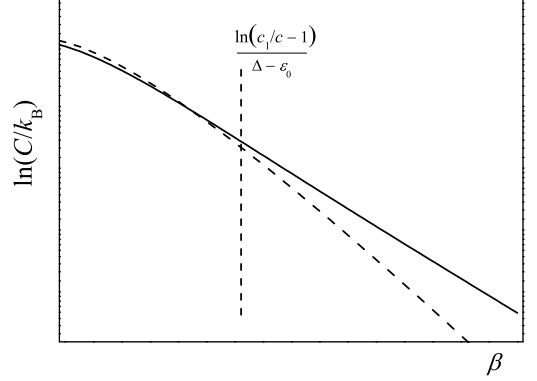


FIG. 8: Temperature behavior of specific heat for a SC with impurities presents a crossover from $\beta\Delta$ exponent (dashed line) to $\beta\varepsilon_0$ at low enough temperature (high enough $\beta = 1/k_B T$).

31]. In that approximation, the only perturbation parameter is the (constant) quasiparticle lifetime τ . In our framework, the τ^{-1} can be related to $\operatorname{Im}\Sigma(\varepsilon)$ at a proper choice of energy, $\varepsilon \sim |\Delta - \varepsilon| \sim \Delta$. Then, in the self-consistent T-matrix approximation [24], we estimate $\tau^{-1} \sim c\Delta/c_1$ which leads to the relation $\tau T_c \sim c_1/c$, reaching at $c \gtrsim c_1$ a qualitative agreement with the Abrikosov-Gor'kov universal criterion for complete SC suppression $\tau T_c < 0.567$ (though in our case this criterion is not universal and depends yet on the perturbation parameter v).

Finally, a similar analysis can be applied for the impurity effect on the electronic specific heat in the SC state, whose dependence on inverse temperature $\beta = 1/k_B T$ is represented as:

$$C(\beta) = \frac{\partial}{\partial T} \int_0^\infty \frac{\rho(\varepsilon) d\varepsilon}{e^{\beta\varepsilon} + 1}, \quad (44)$$

and naturally divided in two characteristic contributions, $C = C_i + C_b$, from ρ_i and ρ_b states:

$$C_i(\beta) \approx k_B c \left[\frac{\beta\varepsilon_0}{2 \cosh(\beta\varepsilon_0/2)} \right]^2,$$

and

$$C_b(\beta) \approx k_B (c_1 - c) v (\beta\Delta_c)^{3/2} \exp(-\beta\Delta_c).$$

The resulting function $C(\beta)$ deviates from the known low temperature behavior $C_0(\beta) \sim \exp(-\beta\Delta)$ for non-perturbed SC system at $\beta > \ln(c_1/c - 1)/(\Delta - \varepsilon_0)$, where the characteristic exponent is changed to a slower $\sim \exp(-\beta\varepsilon_0)$ as seen in Fig. 8.

The same approach can be used for calculation of other observable characteristics for SC state under impurity effect, such as, e.g., differential conductivity for scanning

tunneling spectroscopy or absorption coefficient for far infrared radiation, though these issues are beyond the scope of this work.

VII. CONCLUSIONS

Resuming, the Green function analysis of quasiparticle spectra in an SC ferropnictide with impurities permits to describe formation of impurity localized levels within SC gap and, with growing impurity concentration, of specific

band of extended quasiparticle states, mainly supported by impurity centers. Explicit dispersion laws and densities of states are obtained for modified main bands and impurity bands. Further specification of the nature of all the states in different energy ranges within the SC gap is attained with analysis of group expansions for self-energy matrix, resulting in criteria for crossovers between localized and extended states. The developed spectral characteristics are applied for description of observable impurity effects.

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